

Robust Summaries for

Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene)

CAS No. 10595-60-5

Existing Chemical ID: 10595-60-5
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Producer Related Part
Company: PPG Industries, Inc.
Creation date: 01-NOV-2002

Substance Related Part
Company: PPG Industries, Inc.
Creation date: 01-NOV-2002

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Reliability (profile): Reliability: without reliability, 1, 2, 3, 4

Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2. Physico-chemical Data

date: 12-Aug-2003
Substance ID: 10595-60-5

2.1 Melting Point

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2.2 Boiling Point

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2.4 Vapour Pressure

Value: = .00035 hPa at 25 degree C

Method: other (calculated)
Year: 2002
GLP: no

Remark: The vapor pressure was estimated using the EPIWIN/MPBPWIN Program. The calculation used a boiling point of 321.28 degree C that was calculated by the same model. The vapor pressure calculation was done by the modified Grain method.

Reliability: (2) valid with restrictions
Data were obtained by modeling.

2.5 Partition Coefficient

Partition Coeff.: octanol-water
log Pow: = 7.63

Method: other (calculated)
Year: 2002
GLP: no

Remark: The Log Kow was calculated using the EPIWIN/WSKow program.

Reliability: (2) valid with restrictions
Data were obtained by modeling.

2.6.1 Solubility in different media

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3. Environmental Fate and Pathways

3.1.1 Photodegradation

Type: air
Light source: other
DIRECT PHOTOLYSIS
Half-life t_{1/2}: = .1 day(s)

Method: other (calculated)
Year: 2002
GLP: no

Method: The half-life is calculated using the EPIWIN/AOPWIN Program.
The hydroxyl radical rate constant was calculated to be
95.2679 E-12 cm³/molecule-sec.

Reliability: (2) valid with restrictions
Data were obtained by modeling.

3.1.2 Stability in Water

Type: abiotic
t_{1/2} pH4: = 34.0 minute(s) at 20 degree C
t_{1/2} pH7: = 5.04 minute(s) at 20 degree C
t_{1/2} pH9: = 0.972 minute(s) at 20 degree C
t_{1/2} pH 1.2 : = 51.2 minute(s) at 20 degree C
Deg. products: yes
108-10-1 203-550-1 4-methylpentan-2-one
111-40-0 203-865-4 2,2'-iminodi(ethylamine)

Method: OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year: 2003
GLP: yes
Test substance: other TS

Result: The temperature of the test solutions was maintained at
approximately 20 degree C during hydrolysis testing. The pH
of the test solutions was relatively unchanged. The test
substance hydrolyzed rapidly in natural water bodies. In
addition, the presence of the degradate DETA was confirmed
during each of the tests.

Test condition: Hydrolysis testing was performed at approximately 2450 mg/L at
pH 1.2 and 4 and approximately 250 mg/L at pH 7 and 9.
Samples were collected at four to six intervals, depending on
pH, to monitor a fast hydrolysis rate. At each interval, the
concentration of the test substance and the presence of the
degradate diethylenetriamine (DETA, CAS number 111-40-0) in
solution was determined by liquid chromatography/mass
spectrometry (LC/MS).

Test substance: The test substance used was 70% diethylenetriamine,
1,7-bis(1,3-dimethylbutylidene) in methylisobutylketone
(MIBK). The reference substance used was Diethylenetriamine
(DETA, CAS number 111-40-0).

3. Environmental Fate and Pathways

Reliability: (1) valid without restriction

Reference: (1)

Type: abiotic
t1/2 pH4: < 5 minute(s) at 20 degree C
t1/2 pH7: < 5 minute(s) at 20 degree C
t1/2 pH9: < 5 minute(s) at 20 degree C
t1/2 pH 1 : < 5 minute(s) at 20 degree C
Deg. products: yes
108-10-1 203-550-1 4-methylpentan-2-one
111-40-0 203-865-4 2,2'-iminodi(ethylamine)
Method: OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year: 2002
GLP: no
Test substance: other TS

Result: Over 90 % of the test substance hydrolyzed within 5 minutes. The test substance was almost completely hydrolyzed within one hour period. The presence of the degradate DETA was also confirmed.

Test condition: Hydrolysis testing was performed with test substance in 0.01 molar at pH 1, 4, 7, and 9. Samples were collected at the very beginning of the reaction and at several successive intervals. At each interval, the concentration of the test substance and the presence of the degradate diethylenetriamine (DETA, CAS number 111-40-0) in solution was determined by mass spectrometry (MS).

Test substance: The test substance used was 70% diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene) in methylisobutylketone (MIBK). The reference substance used was Diethylenetriamine (DETA, CAS number 111-40-0).

Reliability: (2) valid with restrictions
The test was not conducted in compliance with GLP.

Reference: (2)

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: water - air
Method: other
Year: 2002
Air: .078 % (Fugacity Model Level I)
Water: 3.59 % (Fugacity Model Level I)
Soil: 27.3 % (Fugacity Model Level I)

Method: The EPIWIN Program was used to conduct Level III fugacity modeling. A mass amount of 69% is estimated for sediment using the same model.

Reliability: (2) valid with restrictions
Data were obtained by modeling.

3. Environmental Fate and Pathways

date: 12-Aug-2003
Substance ID: 10595-60-5

3.5 Biodegradation

4. Ecotoxicity

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

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4.2 Acute Toxicity to Aquatic Invertebrates

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4.3 Toxicity to Aquatic Plants e.g. Algae

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5. Toxicity

date: 12-Aug-2003
Substance ID: 10595-60-5

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain: other
Sex: male/female
No. of Animals: 30
Doses: 1.0, 2.0, 4.0 ml/kg
Value: = 1.9 ml/kg bw

Method: other
Year: 1981
GLP: no
Test substance: as prescribed in the test plan

Method: Standard FHSA procedures was followed.
Result: All animals dosed at 4.0 ml/kg died within one day of dosing. Six animals died from one to nine days after dosing in the 2.0 ml/kg group. No animals treated with 1 ml/kg died. The LD50 was 2.13 ml/kg for males, 1.64 ml/kg for females, and 1.88 ml/kg for both sexes.
Test condition: Groups of five male and five female fasted Albino rats were dosed with the undiluted sample at dosage levels of 4, 2, and 1 ml/kg. Animals were observed for signs of toxicity and mortality. Weight changes were measured in 14 day study period. Necropsies were performed on all animals upon death or 14 days after dosing.
Reliability: (2) valid with restrictions
The test was not conducted in compliance with GLP. The study is comparable to a Guideline study and is acceptable for assessment.

Reference: (3)

5.1.2 Acute Inhalation Toxicity

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5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain: New Zealand white
Sex: male/female
No. of Animals: 4
Doses: 2.0 ml/kg
Value: > 2 ml/kg bw

Method: other
Year: 1981
GLP: no
Test substance: as prescribed in the test plan

5. Toxicity

Method: Modified Interagency Regulatory Liason Group Guidelines for Selected Acute Toxicity Test.

Result: No animals died during the 14 day test period. Severe erythema, severe eschar, and necrosis were noted. The LD50 was greater than 2 ml/kg body weight.

Test condition: Dorsal area (240 cm²) of two males and two females was abraded and dosed under porous gauze dressing covered by a semi-occlusive wrapping of polyethylene sheetings. Rabbits were restrained in a hood for 24-hour contact period.

Reliability: (2) valid with restrictions
The test was not conducted in compliance with GLP.

Reference: (3)

5.1.4 Acute Toxicity, other Routes

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5.4 Repeated Dose Toxicity

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5.5 Genetic Toxicity 'in Vitro'

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5.6 Genetic Toxicity 'in Vivo'

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5.8.1 Toxicity to Fertility

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5.8.2 Developmental Toxicity/Teratogenicity

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9. References

- (1) Springborn Smithers Laboratories. Report 511.6215, Dated 10-29-02.
- (2) PPG Industries Analytical Report No. CR10040, Dated 9-18-02.
- (3) Carnegie-Mellon Institute of Research Report No. 81-21S, Dated 3-13-81.